

# Ferromagnetism in repulsive Fermi gases: upper branch of Feshbach resonance versus hard spheres

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We use quantum Monte Carlo, including backflow corrections, to investigate a two-component Fermi gas on the upper branch of a Feshbach resonance and contrast it with the hard sphere gas. We find that, in both cases, the Fermi liquid becomes unstable to ferromagnetism at a  $k_F a$  smaller than the mean field result, where  $k_F$  is the Fermi wavevector and  $a$  the scattering length. Even though the total energies  $E(k_F a)$  are similar in the two cases, their pair correlations and kinetic energies are completely different, reflecting the underlying potentials. We discuss the extent to which our calculations shed light on recent experiments.

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**Introduction:** Ultracold atomic gases are emerging as a unique laboratory for testing quantum many-body Hamiltonians. A problem of fundamental importance is the ground state of two species of fermions interacting via *repulsive* interactions. The attractive case is now well-understood and shows the BCS-BEC crossover [1] in the superfluid ground state. The broken symmetry is already apparent within BCS mean field theory (MFT) with an arbitrarily small attraction leading to a paired superfluid. In contrast, we know much less about the repulsive case. The Landau Fermi liquid, known to exist at weak repulsion [2], can become unstable only beyond a critical value of the interaction [3]. Thus the phase transition is *not* a weak coupling problem, and the validity of MFT in the repulsive case is questionable.

An exciting new development is a recent experiment [4] which has been interpreted as evidence for a ferromagnetic instability [3, 5–7] in a “repulsive” Fermi gas of  $^6\text{Li}$  atoms. A crucial point is that the interactions between the atoms are quite different from the textbook problem of hard-sphere interactions. In the experiment, the atoms are on the *upper branch* of a Feshbach resonance with a positive s-wave scattering length  $a$ . The two-body ground state then is a molecule of size  $a$ . But in the upper branch, where the wave function is made up from scattering states, the atoms feel an *effective repulsion* characterized by  $a > 0$ , despite the fact that the underlying potential is attractive.

The main question we examine in this Letter is the extent to which the many-body physics in the upper branch is similar to, or different from, that of a purely repulsive Fermi gas. We use quantum Monte Carlo (QMC) to compute the energy, chemical potential and pair distribution function of the two systems – upper branch and repulsive – to understand the instability of the Fermi liquid to ferromagnetism. We believe that such a study of equilibrium properties is necessary, before one addresses non-equilibrium questions in the upper branch.

Before describing our results, we emphasize important ways in which our work differs from previous studies,

which focus on MFT of purely repulsive interactions. First, we carefully discuss what it means for a many-body wavefunction to be on the upper branch, which is essential to describe the experiments. Second, it is crucial to use QMC for this strong coupling problem. For instance, QMC calculations [8] for the electron gas show that ferromagnetism sets in at a critical density nearly 3 orders of magnitude smaller than that predicted by Hartree-Fock MFT. Finally, we include backflow corrections, which can have a nontrivial effect on the nodes of the many-body wavefunction, and thus on the ground state energy [9]. Not including backflow may lead to spurious ferromagnetic instabilities in normal  $^3\text{He}$  [10].

Our main results are that we find Ferromagnetic (FM) instabilities in both the upper branch and the hard sphere Fermi gas. For small  $k_F a > 0$ , with  $k_F$  the Fermi wavevector and  $a$  the s-wave scattering length, both systems are Landau Fermi liquids. The upper branch becomes unstable to a FM state at  $k_F a = 0.89(2)$ , independent of the details of the interaction (in the zero-range limit). The critical  $k_F a$  is similar for a purely repulsive interaction, but the result is *non-universal* and depends on details the potential; we will focus on hard spheres of diameter  $a$ . In both cases the critical value is considerably smaller than the Stoner MFT result  $(k_F a)_{\text{MFT}} = \pi/2$  [3]. Despite similar values of the critical interaction, the behavior of the kinetic energy and the two-body correlations are *qualitatively different* for the upper branch and hard spheres. We also discuss the harmonically trapped gas using the local density approximation (LDA). We conclude with a brief comparison of our results with experiments [4]. We find that some aspects of the experiment cannot be understood within our equilibrium theory.

**Model:** We consider a gas of  $N = (N_\uparrow + N_\downarrow)$  fermions of mass  $m$  with two species, denoted by “spin”  $\uparrow$  and  $\downarrow$ , which interact via a potential  $V(r)$ . The Hamiltonian is

$$H = \sum_{i\sigma} \frac{\mathbf{p}_{i\sigma}^2}{2m} + \frac{1}{2} \sum_{i,j} V(r_{ij}) \quad (1)$$

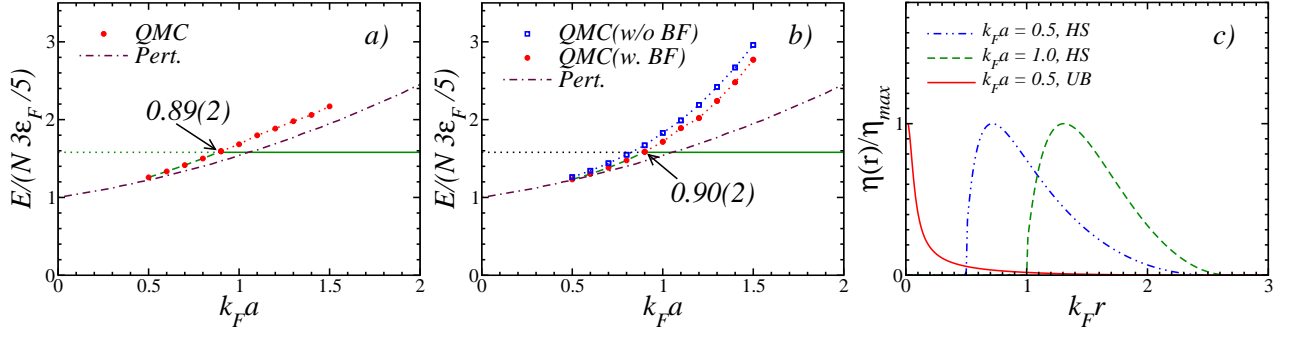


FIG. 1: (Color online) QMC energy per particle for the Fermi liquid state (for  $N_\uparrow = N_\downarrow = 33$  particles) as a function of  $k_F a$  for (a) the upper branch and for (b) hard spheres, compared with the perturbative result Eq. (3). Panel (b) shows QMC with and without backflow (BF) corrections. Backflow does not have a significant effect on the upper branch results in (a). There is a transition to a ferromagnetic state when the QMC energy crosses that of the fully polarized gas (horizontal lines). (c) The function  $\eta(r)$  describing BF correlation, discussed in the text, for the upper branch (UB) and hard sphere (HS) gas.

with  $r_{ij} = |\mathbf{r}_{i\uparrow} - \mathbf{r}_{j\downarrow}|$ . For the QMC calculations we consider a cubic box with periodic boundary conditions. (At the end, we also discuss trap effects within LDA). We measure lengths in units of  $k_F^{-1}$ , where  $k_F = (3\pi^2 n)^{1/3}$  for a free Fermi gas of density  $n$ . We measure energies in units of  $\epsilon_{FG} = 3\epsilon_F/5$  where  $\epsilon_F = k_F^2/2m$  (with  $\hbar = 1$ ).

We consider two forms of the interaction potential. For the repulsive case, we use  $V(r) = V_0 > 0$  for  $r < R$  and zero elsewhere. In the hard sphere limit  $V_0 \rightarrow \infty$  and the diameter of the sphere  $R = a$  scattering length. For the attractive case, we use  $V(r) = -(8/mR^2)V_0/\cosh^2(2r/R)$ , extensively used in BCS-BEC crossover studies [11, 12]. We choose the range such that  $k_F R \ll 0.1$ , so that we obtain universal results independent of the detailed form of  $V(r)$ . We use  $V_0$  to tune the scattering length  $a > 0$ , such that  $V(r)$  has a single bound state. We will focus on scattering states to construct the upper branch wavefunction.

**QMC Results:** The many-body wave function for a (paramagnetic) Fermi liquid is of the Jastrow-Slater form

$$\Psi = \prod_{i\uparrow, j\downarrow} f(r_{ij}) \Phi_{FG\uparrow} \Phi_{FG\downarrow}. \quad (2)$$

The Slater determinants  $\Phi_{FG\sigma}$ 's are constructed from plane waves, and the symmetric Jastrow function  $f(r)$  accounts for interactions.

We now argue that the upper branch Jastrow factor must be qualitatively different from the  $f(r) \geq 0$  used for the purely repulsive case. To see this, consider using a conventional nodeless  $f(r)$  for the attractive Fermi gas. This state is a *normal* Fermi liquid, and thus orthogonal (for large  $N$ ) to the *superfluid* ground state [1, 11] of the BCS-BEC crossover for all  $k_F a$ . However, the energy per particle in this state is always *lower* than the free gas  $3\epsilon_F/5$ , which means that the fermions do feel an attraction. In other words, this normal wave function necessarily has some pairing (bound state-like) correlations, and is therefore *not* on the upper branch.

A necessary condition for a many-body state to be on the upper branch is that its energy per particle must be greater than  $3\epsilon_F/5$ . We must ensure that every pair of particles feels an effective repulsion. We achieve this by introducing a node in the Jastrow  $f(r)$ . To determine  $f(r)$ , we use the lowest-order constrained variational (LOCV) method [13], which is well known in nuclear physics and has also been used for strongly interacting quantum gases [12, 14]. The LOCV equation has an upper-branch solution [15]  $f(r)$  with a node, whose location tracks the scattering length at small  $a$  [i.e.,  $f(r) \sim (1 - a/r)$ ] but then saturates at large  $a$ .

We use QMC to calculate the energy for the upper branch [Fig. 1(a)] and the hard sphere Fermi gas [Fig. 1(b)] with  $N_\uparrow = N_\downarrow$ . For small  $k_F a$ , both results agree with the well-known perturbative result [2]

$$\frac{E}{N\epsilon_F} = \frac{3}{5} + \frac{2}{3\pi} k_F a + \frac{4}{35\pi^2} (11 - 2\ln 2) (k_F a)^2 + \dots \quad (3)$$

We note that Eq. (3) should be taken seriously *only* for  $k_F a \ll 1$ ; the third order term is known to be *non*-universal, and depends on the detailed shape of the potential and on the p-wave scattering channel [2].

A sufficient criterion for ferromagnetism (FM) is that the energy of the paramagnetic Fermi liquid state exceed that of the fully polarized state  $\epsilon_{FG}^P/(3\epsilon_F/5) = 2^{2/3} \simeq 1.58$ . It is instructive to begin with simple analytical approximations (even though these involve using Eq. (3) beyond its domain of validity!) The simplest approximation is to just keep the first term in (3), the mean field Hartree shift. We find that this energy crosses that of the fully polarized  $\epsilon_{FG}^P$  at  $k_F a = (2^{2/3} - 1)9\pi/10 \simeq 1.66$ . This is slightly larger than the Stoner estimate of  $\pi/2$ , but still below the hard sphere solidification limit  $k_F a = (9\pi/4)^{1/3} \simeq 1.92$ . Including the second order term in (3) increases the energy of the paramagnetic Fermi-liquid solution, and thus FM sets in closer to  $k_F a \simeq 1$ .

The QMC energy for both the upper branch and hard

spheres implies a FM ground state for  $k_F a \gtrsim 0.9$ . We next address backflow to see how it affects our conclusion. **Backflow:** It is very important to include backflow which, as noted above, makes nontrivial modifications to the nodal surfaces and can lead to large quantitative effects [9] in the ground state energy. Backflow modifies the single-particle plane wave orbitals  $\phi_{\mathbf{k}}(\mathbf{r}_{i\sigma}) = \exp[i\mathbf{k} \cdot \mathbf{r}_{i\sigma}]$  used to construct the Slater determinants in Eq. (2) via the replacement  $\mathbf{r}_{i\sigma} \rightarrow \mathbf{r}_{i\sigma} + \sum_j \eta(r_{ij})\mathbf{r}_{ij}$ , where  $j$  labels particles of the opposite spin  $\bar{\sigma}$ .

The optimal form of the backflow function  $\eta(r)$  must be determined for each problem; it is known to be very different for the  $^4\text{He}$  roton [16], for normal  $^3\text{He}$  [17], and for the electron gas [18]. Insight into the form of  $\eta(r)$  for  $^3\text{He}$  came from analyzing the problem of a  $^3\text{He}$  impurity in  $^4\text{He}$  [17]. Following the same logic, we consider a single spin-down impurity in a spin-up Fermi sea. Omitting the details of our analysis (which will be reported elsewhere), we find the  $\eta(r)$ 's shown in Fig. 1(c).

For the hard sphere gas the optimal  $\eta(r)$  vanishes inside the hard-core diameter and has a single peak just beyond it, qualitatively similar to the case of  $^3\text{He}$  [9, 17]. As in  $^3\text{He}$ , we approximate the form of  $\eta(r)$  by a Gaussian whose parameters we optimize. We use QMC to compute the energy of hard spheres using Eq. (2) with a nodeless Jastrow times backflow-corrected Slater determinants. We find that backflow leads to a significant lowering of energy [see Fig. 1(b)] that becomes more pronounced with increasing  $k_F a$ . For example, there is a 5.5% reduction in energy at  $k_F a = 1$ .

For the upper branch, we find that the form of the optimal  $\eta(r)$  is qualitatively different; see Fig. 1(c). It is nonzero at the origin and decreases monotonically, with a power-law decay at large  $r$ . Further,  $\eta(r)$  changes very little with  $k_F a$  compared with the hard sphere case. The form of upper branch  $\eta(r)$  is similar to systems with a soft-core, long-range repulsion, like the electron gas [18]. We use QMC to calculate the energy of the upper branch state (2), with a Jastrow with a single node, times backflow-corrected Slater determinants. In this case the reduction in energy is small [Fig. 1(a)] and falls within our statistical error of  $\lesssim 1\%$ .

We thus find that backflow is important for hard spheres when  $k_F^{-1}$  is comparable to the hard-core diameter  $R = a$ . On the other hand, backflow effects are small for the upper branch, where  $k_F^{-1} \gg R$ , the range.

**Observables:** For both the upper branch and for hard spheres, we conclude that ferromagnetism is energetically favorable, based on the crossing of energies of the paramagnetic Fermi liquid and the fully polarized FM; see Fig. 1(a,b). For the upper branch, we find that FM state is stable for  $k_F a \geq 0.89(2)$ . The order of the transition requires a careful finite-size scaling analysis in the vicinity of the phase transition, beyond the scope of our present investigation.

Although the total energies in the Fermi liquid phases

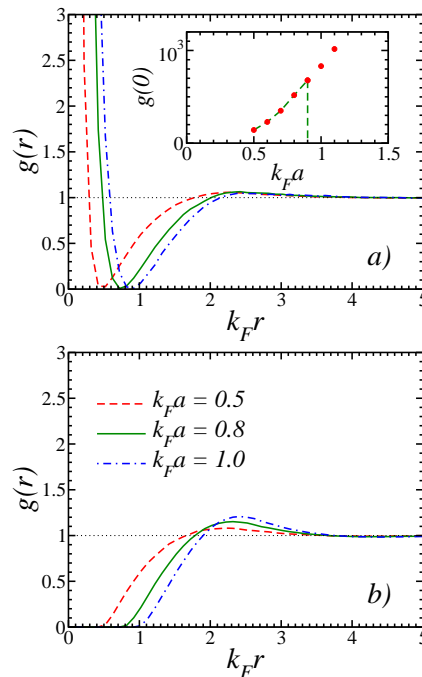


FIG. 2: (Color online) Pair distribution function  $g(r) \equiv g_{\uparrow\downarrow}(r)$  for (a) the upper branch and (b) the hard sphere gas for various values of  $k_F a$ . Inset in panel (a) shows  $g(r=0)$  as a function of  $k_F a$ .

in the upper branch and hard spheres are similar, the potential  $\langle V \rangle$  and kinetic energy  $\langle K \rangle$  are very different in the two cases. To understand this, it is illuminating to look at the pair distribution function  $g_{\uparrow\downarrow}(r)$ , denoted by  $g(r)$  for simplicity. In the hard sphere case [Fig. 2(b)],  $g(r)$  vanishes inside the hard-core and goes to unity at large separation. The potential energy  $\langle V \rangle \sim \int d^3\mathbf{r} g(r) V(r)$  then vanishes identically and the total energy [Fig. 1(b)] in the hard sphere case is entirely kinetic.

In the upper branch, on the other hand, we find a large cancellation between a positive  $\langle K \rangle$  and a negative  $\langle V \rangle$ . In marked contrast to hard spheres, the upper branch  $g(r)$  is extremely large at  $r = 0$ , has a pronounced dip at the node in the Jastrow  $f(r)$  and then goes to unity at large  $r$ ; see Fig. 2(a). For the short-range attraction, the potential energy  $\langle V \rangle \sim g(0) \int d^3\mathbf{r} V(r)$  is thus large and negative, dominated by the growth of  $g(0)$  with increasing  $k_F a$  [inset of Fig. 2(a)]. This is compensated by a large positive kinetic energy  $\langle K \rangle$  [Fig. 3(a)] so that we find the total energy shown in Fig. 1(a).

**Harmonic Trap:** We first obtain from our QMC data the chemical potential  $\mu = (\partial E / \partial N)$  as a function of density [Fig. 3(b)]. We then invert this to find the equation of state  $n(\mu)$  of the *homogeneous* system.

We restrict ourselves to the paramagnetic Fermi liquid regime here, and use the LDA  $\mu(r) = \mu(0) - V_{\text{trap}}(r)$  to study the effects of the harmonic trap  $V_{\text{trap}}(r)$  with associated length scale  $a_{HO}$ . To compare with experiments,

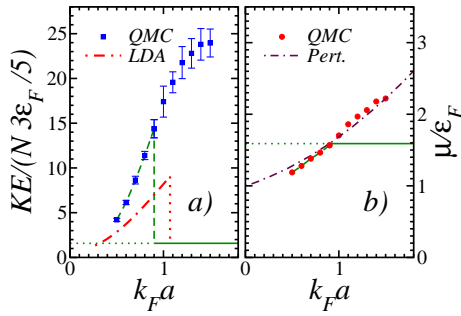


FIG. 3: (Color online) (a) Kinetic energy (KE) per particle of the upper branch. Squares represent QMC data as a function  $k_F a$ . The dashed line at  $k_F a = 0.89$  shows the ferromagnetic transition at which the KE is greatly suppressed and then remains constant. The dot-dash curve is the LDA result for the KE versus  $k_F^0 a$  using the QMC equation of state. Within LDA, ferromagnetism appears at the center of the trap when  $k_F^0 a \simeq 1.1$ . (b) Chemical potential  $\mu(k_F a)$ , related to the square of the LDA radius of the trapped cloud, for the upper branch. The perturbative result for  $\mu = (\partial E / \partial N)$  obtained from Eq. (3) is also shown.

we use the parameter  $k_F^0 = (24N)^{1/6} / a_{HO}$  as a measure of the total number of particles  $N$ . To find the LDA equation  $(k_F a)^6 = 2^{3/2} 48\pi \int_0^{\tilde{\mu}(0)} d\tilde{\mu} [\tilde{\mu}(0) - \tilde{\mu}]^{1/2} \tilde{n}(\tilde{\mu})$ . Here we have used dimensionless quantities  $\tilde{\mu} = \mu(0) m a^2$  and  $\tilde{n}(\tilde{\mu}) = n(\mu) a^3$ , where  $n(\mu)$  is the QMC equation of state.

We then find the density  $n(r = 0)$  at the center of the trap, from which we can determine the interaction parameter  $k_F(0)a = [3\pi^2 \tilde{n}(\tilde{\mu}(0))]^{1/3}$ . We find that for  $k_F^0 a \simeq 1.1$ , the trap center reaches  $k_F(0)a = 0.89$ , the critical value in the homogeneous case. At this point the center of the trap should become unstable to ferromagnetism. We have also calculated within LDA the total and kinetic energies in the trapped system as functions of  $k_F^0 a$ ; the latter is shown in Fig. 3(a).

**Comparison with experiments:** While we were motivated by the experiments of Ref. [4], we focus only on “equilibrium” in the upper branch, and do not address dynamical questions. If three-body processes leading to molecule formation can be suppressed, there may be a window of time-scales where equilibrium physics in the upper branch, as described here, would be observed. The  $k_F a$ -dependence of  $g(r = 0)$  [inset of Fig. 2(a)] is relevant to the loss rate [19] due to molecule formation.

Even with these caveats, there are some aspects of the experiment which we can understand qualitatively and others we cannot. First, we do find a ferromagnetic instability in the upper branch, but predict that it should happen in a homogeneous system at  $k_F a = 0.89$ , which translates into the onset of FM at the center of the trap at  $k_F^0 a \simeq 1.1$ , while the experiment sees interesting features only at  $k_F^0 a \simeq 2$ . The behavior of the chemical potential [Fig. 3(b)], which increases with increases  $k_F a$  and then

saturates beyond the transition is qualitatively consistent with the experiment. However, the  $k_F a$ -dependence of the kinetic energy is not; our results in Fig. 3(a) are qualitatively different from the experiments. Finally, we have not addressed here the question of FM domains and their sizes, which is important to understand given that they have not been seen in the experiment.

**Conclusions:** We show using QMC that fermions with effectively repulsive interactions become unstable to ferromagnetism beyond a critical interaction strength  $k_F a \simeq 0.9$ . This is true both for fermions in the upper branch (scattering state with positive  $a$ ) of an attractive potential and also for hard sphere repulsion, despite important differences in their short range correlations and the kinetic energy that reflect the underlying potentials.

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**Note added:** As we were writing this paper, the work of Pilati *et al.* appeared [20]. It addresses the same problem using a similar, but not identical, approach. Wherever they overlap, our results are in essential agreement.

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